

2,2,3-Trimethylbutane
464-06-2 | DTXSID7060047

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.57×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.75×10^{-1}

Confidence level: 7.76×10^{-1}

Nearest Neighbors from the Training Set

Image not found

2,2,3-Trimethylbutane

Measured: 4.23×10^{-12}

Predicted: 3.57×10^{-12}

Image not found

Pentane, 2,2-dimethyl-

Measured: 3.37×10^{-12}

Predicted: 3.83×10^{-12}

Image not found

Butane, 2,2,3,3-tetramethyl-

Measured: 1.08×10^{-12}

Predicted: 2.47×10^{-12}

Image not found

2,3,4-Trimethylpentane

Measured: 6.99×10^{-12}

Predicted: 5.11×10^{-12}

Image not found

2,4-Dimethylpentane

Measured: 5.16×10^{-12}

Predicted: 5.28×10^{-12}